NASA CONTRACT NSR 52-112-001

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Quarterly Status Report of work accomplished during the period 1 January 1967 to 31 March 1967

1. Previous Quarter

In the previous two quarters a programme was developed for computing transport cross sections and collision integrals such as those required on the contract. At the end of the last quarter the programme was finally checked by running it for some potentials for which the cross sections and collision integrals were known. All these tests showed that the programme was working correctly for both repulsive and attractive potentials.

2. Repulsive Power Inverse Potentials

In the present quarter (1 January 1967 to 31 March 1967) the programme was run for the repulsive potentials

$$V(r) = K P / r^{n} \tag{1}$$

for which the collision integrals are given by

$$\Omega^{(l,s)} = \left(\frac{\pi k T}{2\mu}\right)^{\frac{1}{2}}\left(\frac{nC}{kT}\right)^{\frac{2}{n}}\Gamma\left(s+2-(2/n)\right)A^{(l)}(n) \tag{2}$$

and

$$A^{(l)}(n) = \left[\frac{\mu g^{2}}{2nC}\right]^{\frac{2}{n}}\int_{0}^{\infty}\left(1-\cos^{l}\chi\right)b\,db$$

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for the values of n required in the contract n = 2, 3, 4, 5, 6, 8, 10, 15, 25 and 50. The quantities $A^{(}(n)$ were computed from the transport cross sections

$$Q^{(}(E) = 2\pi \int_0^\infty b\,(1 - \cos^{(} \chi)\,db$$

where b is the impact parameter, E is the energy in centre-of-mass coordinates and χ is the classical deflection angle because

$$A^{(}(n) = \left(\frac{E}{nC}\right)^{\frac{2}{n}} \frac{1}{2\pi} Q^{(}(E) \qquad . \qquad (3)$$

To obtain an estimate of the accuracy of our calculations we computed $A^{(}(n)$ from $Q^{(}(E)$ for several energies E. Since $A^{(}(n)$ is independent of E the slight differences between the values of $A^{(}(n)$ computed for different energies gave an estimate of the accuracy of our calculations. The results to the accuracy of our calculations are given in the accompanying table. Also shown are the results of Kihara, Taylor and Hirschfelder[1] in cases where there is overlap between our calculations. The agreement is excellent except at $n = 2$ where disagreement is only a few percent. We are examining this small disagreement at present by increasing the number of quadrature points, and suspect it might be due to numerical errors in our calculations.

3. Attractive (rigid) Inverse Power Potential

In the previous quarter we had described a method of introducing a rigid core of such a small radius that it had no effect on the calculations for the negative screened Coulomb potential

$$V(r) = -\frac{\rho}{r}\, e^{-(r/\rho)}$$

Although this method worked extremely well for this potential we had great difficulty in using it for the attractive inverse power potentials. We, therefore, have changed the logic of the programme to take account of the form of the potential by calculating χ directly from the formula

$$\chi = \pi - 2b(I_1 + I_2) \tag{4}$$

where
$$I_1 = \int_{r_m}^{r_{max}} \frac{dr/r^2}{F(r)} \tag{5}$$

and
$$I_2 = \int_{r_{max}}^{\infty} \frac{dr/r^2}{F(r)} \tag{6}$$

In these formulas r_m is the outermost zero of $F(r) = [1 - V(r)/E - b^2/r^2]^{\frac{1}{2}}$ and r_{max} is the value of r at which the integrand has a maximum value. This method had been programmed but not fully tested at the end of the quarter.

4. Travel

During this quarter Dr. Smith travelled once to the Institute of Advanced Studies in Dublin and once to Harwell to consult with colleagues on problems related to the work on the contract.

5. Following Quarter (April to June)

The accuracy of the calculations for the repulsive inverse power potentials will be accurately determined. The programme for the attractive inverse power potentials will be finally checked and used to compute the cross sections required in the contract. Difficulty is expected only for the case $n = 2$. The collision integrals for the exponential repulsive potential required in the contract will also be calculated.

A thesis will be completed by Mr. L. D. Higgins, B.A., D.P.E. on material arising from his work on the contract.

Reference

1. T. Kihara, M. H. Taylor and J. O. Hirschfelder, Phys. Fluids 3, 715, (1960).

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Table $A^{(o)}(n, \text{repuls})$

n		$\ell = 1$	$\ell = 2$	$\ell = 3$	$\ell = 4$
2	Hirschfelder	0.3976	0.5278	0.7136	——
	Smith	0.3926	0.518	0.698	0.793
3	Hirschfelder	0.3115	0.3533	0.472	——
	Smith	0.3107	0.3522	0.4704	0.501
4	Hirschfelder	0.298	0.308	——	——
	Smith	0.2983	0.3083	0.4136	0.422
5	Hirschfelder	——	——	——	——
	Smith	0.3000	0.2910	0.3932	0.3888
6	Hirschfelder	0.306	0.283	——	——
	Smith	0.3059	0.2831	0.3854	0.3722
8	Hirschfekder	0.321	0.279	——	——
	Smith	0.3202	0.27784	0.38328	0.35777
10	Hirschfelder	0.333	0.278	——	——
	Smith	0.3338	0.2775	0.38686	0.3528
15	Hirschfelder	——	——	——	——
	Smith	0.36064	0.281403	0.399534	0.35161
25	Hirschfelder	——	——	——	——
	Smith	0.39365	0.29011	0.41966	0.3572
50	Hirschfelder	——	——	——	——
	Smith	0.43103	0.3030	0.4457	0.3687